A Review of Computational Approaches for Chemically Reacting Flows

R. W. Claus
NASA Lewis Research Center, Cleveland, Ohio

INTRODUCTION

Three-dimensional combustor calculations invlove detailed modeling of several important physical processes. Airflow, chemical reactions, fuel sprays, and turbulence are just a few of the physical processes that must be described. Many of these processes occur on both a molecular and a macroscopic scale. To exactly describe these processes numerically, one must resolve these scales on a computational mesh. This is clearly beyound current computational resources. To make the computational task tractable, we introduce modeling assumptions. These modeling assumptions limit the generality of the computational flow code, but it is hoped that the dominant physics remain correctly represented.

Modeling assumptions are only the first limit of generality introduced when developing a combustor flow code. A further limit is introduced by the need to approximate the modeled equations before they are solved numerically. This approximation process can significantly affect the accuracy of a model prediction.

In view of all these factors, a combustor designer cannot be expected to fully embrace a computer model prediction. If a clear distinction between modeling errors and numerical approximation errors cannot be made, then the designer is left with a very unreliable computational tool.

The tremeduous growth in computing power, however, has significantly improved our ability to address these issues. Faster computational speeds and larger memories has permitted the development of more complex turbulence/reaction models and the use of finer computational meshes. As a consequence, a new generation of computational tools are becoming available for the design of both high and low speed combustors. This review will examine some recent improvements in combustion models while noting some of the remaining roadblocks.

Discussion

This review will initially focus on the issues being examined in low speed combustion systems, and then will review some of the work being done for high speed applications. This review is not all inclusive but should be representative of the current state-of-the-art used in combustion system design.

Subsonic Combustion

The lack of shock waves and the frequently imposed assumption that acoustic waves can be neglected, significantly reduces the computational burden for subsonic reacting flows. Before examining reaction models, it is instructive to examine how well a few typical flow fields can be numerically predicted.

A number of alternatives exist to solve the fluid flow equations. The main distinguishing characteristic is how turbulence is represented. The most common approach and the least computationally taxing is to either time or Favre average the Navier Stokes equations. Closure for this class of flow codes employs some type of multi-equation turbulence model, the most common being a two-equation model, ref. 1. Figure 1 displays the results of a three-dimensional flow calculation compared to experimental data. The calculations were made using a two-equation turbulence model for two different geometries. Although the flows are highly similar, the numerical results are significantly different. To examine the effect of mesh refinement, the geometry with the least favorable agreement was used in an extensive mesh refinement study. Figure 2 displays the results of a series of progressively finer meshes. Figure 2a indicates that the mean flow field variables show significant improvement with mesh refinement. The same is true for fluctuating flow quantities as seen in figure 2b. While the trend with mesh refinement is encouraging, it is important to keep in mind the fact that this calculation was for a single, three-dimensional jet-in-crossflow, while a complete combustion system contains many jets and other complex flow features. It is impractical to consider using as many as 2 million mesh points for every complex feature of a typical combustor.

Even if one has sufficient mesh resolution, a two-equation turbulence model is inappropiate for many flows. Figure 3 displays a comparison between a calculated turbulence kinetic energy and experimental data for a two-dimensional, bluff-body, flow field, ref. 2. There is a large region in the flow field where there is a significant discrepancy between experiment and calculation. Mesh refinement does not significantly improve the comparison. The disagreement has been conjectured to be due to large scale vortical structures in the flow field. This bluff body type of flow field is sensitive to instabilities that produce vortical structures that can alter the development of the flow.

Whether or not these structures are defined as turbulence, it is clear that for some flows it is important to include these structures in the calculation. There are two computational alternatives to include these structures. The first, and most practical, is a Large Eddy Simulation (LES). Large Eddy Simulations involve the solution of the time-accurate, Navier Stokes equations to directly resolve the large scale structures and some form of a turbulence model is used to represent more "universal" small scale structures. But even for this class of computations, the lim-

itation remains the turbulence closure used to represent the so-called "universal" small scales. Figure 4 displays the results of a Large Eddy Simulation where both the vortical structure resolved in the calculation and the energy imparted by the turbulence model is shown, ref. 3. The large scale vortices resolved in the calculation agree fairly well with experimental data, but the energy in the turbulence model forms in the incorrect locations. Experimental evidence indicates that the turbulence model should form maximums in the braid region of the vortical structure, but the calculations indicate maximums in the core of the vortices. A second, and less practical approach, to resolve large scale structures is Direct Numerical Simulation (DNS). Direct Numerical Simulations resolve all scales of turbulence on a computational mesh and as a consequence this technique is only applicable for low Reynolds number flows. DNS will not be used to calculate real combustor flow fields, but it may be used to develop more appropriate turbulence models. For example, figure 5 displays the results of a Direct Numerical Simulation where several types of perturbations were added to a flow field to augment the amount of product formed, ref. 4. A dashed type in the figure indicates what would happen if just natural noise was used in the flow. Apparently, the amount of product that is formed can be increased by several factors if the proper forms of forcing are used. In an analogous manner Direct Numerical Simulations can be used to test reaction closures, ref. 5.

Supersonic Combustion

Supersonic combustion certainly imposes severe demands on computational analysis. Although the effect of turbulence may be reduced, ref. 6., it does not go away. Shock waves and the need for detailled finite rate chemistry add large demands for additional mesh resolution and long running times.

A flow field that is analogous to the one examined for subsonic flows is the supersonic jet in cross flow. Figure 6 displays the results of a calculation compared with experimental data from ref. 7. The predictions are for a scalar tracing the jet penetration. The contour level that pentrates the furthest should be compared to the data points. The comparison is very good, but it should be noted that these results are sensitive to mesh refinement. Other flow fields where the blowing rate of the jet is changed are not as well predicted.

With the combined requirement to treat finite rate chemistry and turbulence in compressible flows, Probability Density Function (PDF) methods are being developed for high speed flow codes. Some preliminary calculations, using this technique, have shown very promising results for some simple flows. It remains to be seen if an approach that is this computationally difficult can be usefully included into a design process.

Concluding Remarks

The computational approaches that can be used to calculate both subsonic and supersonic reacting flows have been examined. In general, it has been shown that none of these approaches are perfect, but the technology is rapidly developing. The most promising approaches to improved computational accuracy have been illustrated.

References

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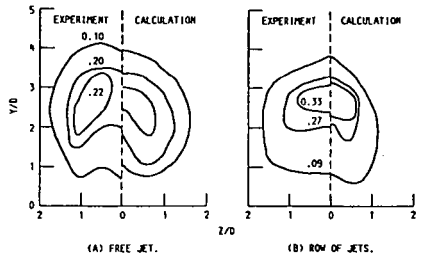
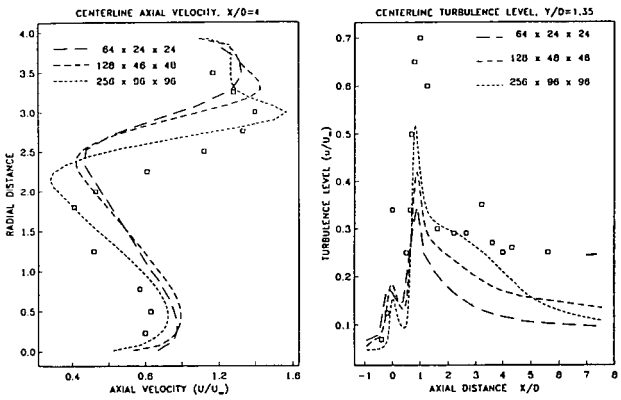


Figure 1. Comparison between experiment and calculation for two parametrically different three-dimensional flow fields.



A) Mean field comparison. B) Turbulence comparison.

Figure 2. The effect of mesh refinement on a comparison with experiemental data for a jet-in-crossflow.

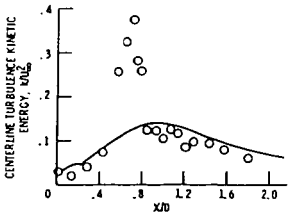
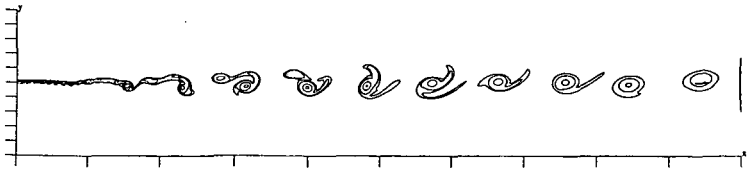
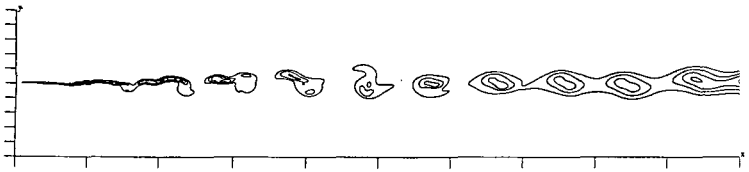


Figure 3. Comparison of a laboratory experiment with numerical prediction for a two-dimensional flow field.



A) Vorticity field.



B) Turbulence kinetic energy.

Figure 4. Results of a Large Eddy Simulation of a forced shear layer.

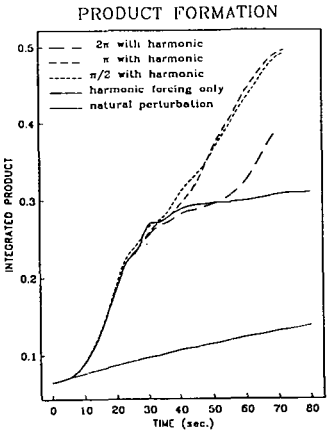


Figure 5. Temporial evolution of the product formed by a perturbed shear layer.

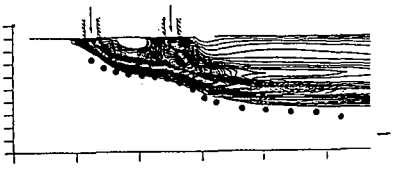


Figure 6. A comparison between predicted and experimental jet penetration in a supersonic flow field.